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X-Division Research Note:

"Investigation of False Learning in Adaptive Monte Carlo Transport"

Abstract

Adaptive Monte Carlo transport relies on learned information to accelerate convergence to a zero-variance biasing solution. Such an iterative procedure is vulnerable to false learning. Any scheme that attempts to avoid such false learning must also avoid precluding zero-variance biasing, which may occur if the scheme is too conservative in it's treatment for undersampled domains of phase space. Hence, a delicate balance between the requisite convergence rate and the all-important correct result must be struck.

This investigation has demonstrated instances of false learning (leading to manifestly incorrect results). It has explored an avoidance [of false learning] approach. And it has identified a potential basis for diagnosing the presence of false learning; namely, a comparison between theoretical and computed values of quantities related to local behavior. Such comparisons recognize that, although the global solution is unknown, local behavior is known. These findings have been based on algorithms applied to discrete state transport scenarios, with an eye toward eventual extension to continuous transport applications.

1. Introduction

This Research Note elaborates a presentation,[1] which was made at a Workshop on Adaptive Monte Carlo Methods.[2] This Workshop was held at Los Alamos National Laboratory (LANL) in August of 1996.

To disambiguate the discussions that follow, it is useful to present several working definitions, in the context of adaptive Monte Carlo:

false learning (FL) – Learning falsely that a domain of phase space is a relatively unimportant contributor to the result; effected by adaptively inadequate sampling. FL can lead to *false convergence*.

false convergence – Convergence to a false result. The opposite of *proper convergence.*

demonstration of FL – Contriving a transport problem that poses a potential FL situation, which requires seemingly heroic *a priori* measures (*i.e.*, ultra conservative initial analog sampling) to avoid false convergence.

avoidance (of FL) strategy – Striving to insure that no sequence of transitions, which could produce significant score, is ignored.

FL diagnostics – Computed feedback that, based on a comparison of known and estimated information, will suggest the presence of FL in the course of a calculation.

In the development of algorithms, two computing tools are often useful – a testbed and a benchmark. The former provides a computational context to test an algorithm's functionality. The latter provides the 'truth' to validate the algorithm's solution.

1.1 Testbed for investigation

In this investigation, the testbed was a multi-state discrete Monte Carlo transport code, written previously by Tom Booth.[3] This code adaptively iterates to zero-variance biasing[4] for transition from state$_i$ to state$_j$, *viz.*

$$q_{ij} = C_i p_{ij}(s_{ij} + m_j) \tag{1}$$

where

q_{ij} is the zero-variance-biased transition (or termination) probability (state$_i$ to state$_j$);

p_{ij} is the unbiased (analog) transition (or termination) probability;

s_{ij} is the associated transition (or termination) score;

m_j is the estimated mean for state$_j$;

C_i is the normalization for state$_i$.

Note that for termination state$_0$ (*i.e.*, the graveyard), $m_0 = 0$.

1.2 Benchmark for investigation

To serve as benchmark, a code[5] was written[†] that computes analytic values of the means corresponding to the multi-state discrete Monte Carlo transport testbed. The analytic values are based on the iteration of:

$$m_i = \sum_{j=0}^{n} p_{ij}(s_{ij} + m_j) \tag{2}$$

where n is the number of states specified, and state$_0$ is the graveyard.

[†] As listed in Ref.[5], the source code contains a bug that was subsequently fixed.

This benchmark code computes analytic values within the machine *double* precision, using an internally computed criterion, *viz.*

```
      subroutine epsil
      implicit double precision (a-h,o-z)
      common/epsilon/eps
c------ compute machine epsilon;
      eps=1.
      do 10 i=1,1000
      if(1.0+eps.eq.1.0)go to 20
10    eps=eps/2.0
20    eps=2.0*eps
      write(*,*)'machine epsilon=',eps
      return
      end
```

On a machine with 32-bit wordsize, the computed double precision is:

$$\epsilon = 2.2 \times 10^{-16} \tag{3}$$

2. Demonstration of False Learning

Recall that zero-variance-biased transition probabilities (beyond the initial iteration) are given by Equation 1:

$$q_{ij} = C_i p_{ij}(s_{ij} + m_j)$$

and that $m_0 = 0$. For a 2-state problem (with the source in state$_1$), it is straightforward to formulate a prescription for a scenario that is susceptible to FL, *viz.*

- Choose p_{12}, p_{21}, and s_{21} such that their product represents a *rare-analog* sequence of transitions, but having a *non-trivial* expected score.
- Contrive to estimate $q_{12} = 0$ after the initial iteration. This can result from:
  - setting $s_{12} = 0$;
  - estimating $m_2 = 0$ in the first iteration, which (given a first batch of histories too small to overcome the odds) can result from:
    * setting $s_{20} = s_{22} = 0$;
    * setting $p_{12} \ll p_{10} + p_{11}$ and $p_{21} \ll p_{20} + p_{22}$.

In accordance with the above prescription, we contrive a 2-state problem (source in state$_1$ and graveyard in state$_0$), having the following transition probabilities and associated scores:

TABLE I
Specification
2-State Problem Susceptible to FL
Source in state_1; graveyard in state_0

	state_0		state_1		state_2	
state_i	p_{i0}	s_{i0}	p_{i1}	s_{i1}	p_{i2}	s_{i2}
state_1	.990	1	.009	1	.001	0
state_2	.990	0	.001	1×10^6	.009	0

Using the 2-state problem specification in Table I, the testbed and benchmark computed results are presented in Table II below. The initial iteration for the testbed calculation used unbiased (analog) transition probabilities.

TABLE II
Computed Results
2-State Problem Susceptible to FL
Source in state_1; graveyard in state_0

Initial histories	Final m_1	Final m_2	False learning	Convergence
10^6 *insufficient!*	1.0081 $\pm$ .0001	*no estimate!*	initial $m_2 = 0$ $\Rightarrow q_{12} = 0$	FALSE
10^7 *heroic?*	2.0263 $\pm$ .0003	1009.1 $\pm$ .1	AVOIDED	PROPER
Analytic values	2.02632...	1009.08...	N/A	N/A

Indeed, the results in Table II above are a clear demonstration of FL. With 10^6 histories in the initial iteration, the initial estimate of $m_2 = 0$, which in turn leads to a first estimate of the zero-variance-biased transition probability $q_{12} = 0$; once that biased transition probability has been zeroed-out, there can be no recovery. This outcome leads to a false convergence of $m_1 = 1.0081 \pm .0001$ and $m_2 = 0$ (implied). But, when the number of histories for the initial iteration is increased to 10^7, the calculation results in proper convergence for both means (as verified by the analytic values computed with the benchmark code).

Of course, the Table II annotations "*insufficient!*," "*no estimate!*," and "*heroic?*" are facetious. Since the product $p_{12} \cdot p_{21} = 10^{-6}$, only 1 history (on average) in 10^6 will survive the odds against tallying a score from state_2. It is, therefore, **not** surprising that none did (for an initial iteration of 10^6 histories), nor is it heroic that 10^7 initial histories enabled proper convergence.

3. An Avoidance Strategy

Having easily demonstrated FL, we turn our attention to developing a strategy for FL avoidance. The crux of the matter is to insure that no sequence of transitions, which could produce significant score, is ignored. But such insurance, in a strict sense, is totally impractical for any but the most trivial of systems. There is, however, a pertinent analogy in the search for an exact zero-variance solution. Quoting Eugene Troubetzkoy,[6]

> A case of zero variance is indeed an *optimum optimorum* and is of high theoretical interest. An exact zero-variance solution requires the complete and exact knowledge of the answer to the problem to be solved. Should such a knowledge exist, the Monte Carlo calculation becomes unnecessary. One usually conjectures that an approximate knowledge of the answer, **treated as exact** [*emphasis added by HL*], leads to an approximately optimal solution, or to near zero variance. We are not aware of any serious attempts to prove this conjecture but do not have any reason to doubt it. The existing evidence shows that, indeed, biasing schemes generated this way lead to dramatic improvements in the variance. (See, for instance, Ref.[7].)

The observed analogy is that a useful FL avoidance strategy could be based on the *tendency* to interrogate all of phase space, without regard to analog transition probabilities. Accordingly, the rationale for a strategy may be set forth as follows:

- Need to inspect adequately all states that contribute significant score.
- In general, adequate inspection of all states is impractical.
- A strategy that *tends* to inspect all states may be a useful first step.
- Given a *finite* first iteration, how can unbiased probabilities be modified to display such a tendency?

The choice of strategy that comes to mind is *a priori* learning using uniform-biasing transition probabilities. Hence, Booth's testbed code was modified to accommodate such biasing for the initial iteration; all subsequent iterations would continue with adaptive zero-variance biasing (Equation 1).

3.1 Test strategy scenario

The objective for a scenario to test the avoidance strategy was to quantify and gauge its efficacy, using an unbiased initial iteration for comparison. For specificity, a sequence of tests was defined, with increasing number of states (n), having tight coupling between contiguous state numbers ($\text{state}_i,\ i = 1, n$):

- Restrict transitions to a contiguous state or termination only, with source in state_1 and termination in graveyard state_0.

- Disallowing other (including in-state) transitions merely accelerates testing.
- Assign $p_{ij} = .1$ probability for all state$_i$-to-state$_j$ transitions, $i \neq j$.
- Assign remaining probability to termination; $p_{i0} = .9$ for an 'end' state (*i.e.*, state$_1$ and state$_n$) or $p_{i0} = .8$ for an 'interior' state.
- For source state$_1$, assign score $s_{10} = 1$ for termination; score $s_{12} = 0$ for transition to state$_2$.
- For every state$_j, j > 1$, assign score $s_{j,j-1} = 100$ for 'downscattering' to state$_{j-1}$; $s_{j0} = s_{j,j+1} = 0$ score otherwise.

A medium so defined is relatively opaque to arrival at higher-number states. Since the higher-number states contribute significant score (upon 'downscattering'), such a medium poses difficulty for FL avoidance. The state-to-state matrix for $n = 6$ is given in Table III below.

TABLE III
6-State Scenario State-to-State Matrix
Source in state$_1$; graveyard in state$_0$

	state$_0$		state$_1$		state$_2$		state$_3$		state$_4$		state$_5$		state$_6$	
state$_i$	p_{i0}	s_{i0}	p_{i1}	s_{i1}	p_{i2}	s_{i2}	p_{i3}	s_{i3}	p_{i4}	s_{i4}	p_{i5}	s_{i5}	p_{i6}	s_{i6}
state$_1$	.9	1	.0	0	.1	0	.0	0	.0	0	.0	0	.0	0
state$_2$	.8	0	.1	100	.0	0	.1	0	.0	0	.0	0	.0	0
state$_3$	.8	0	.0	0	.1	100	.0	0	.1	0	.0	0	.0	0
state$_4$	.8	0	.0	0	.0	0	.1	100	.0	0	.1	0	.0	0
state$_5$	.8	0	.0	0	.0	0	.0	0	.1	100	.0	0	.1	0
state$_6$	.9	0	.0	0	.0	0	.0	0	.0	0	.1	100	.0	0

The "conditions of contest" for this numerical experiment were simple:

1. Seek the threshold number of histories required in the first (*i.e., a priori learning*) iteration to compute a non-zero mean for every state known to have a non-zero mean.
2. Use an incrementing algorithm that tries $10\times$ the number of histories every time a known non-zero mean is computed as zero.

3.2 Test strategy results

The test scenario specified in the preceding section was computed for the cases $n = 2 - 6$. For each case, the crucial comparison was the threshold number of histories in the initial iteration that was required to avoid FL (*i.e.*, learning falsely that a known non-zero mean is zero). The protocol for increasing the number of states n, starting with $n = 2$, was to start each new case with the threshold number of histories for the preceding case (having one fewer state); the starting number for the 2-state case was a mere 10 histories. With each instance of failure to avoid FL, the incrementing algorithm was invoked (see "conditions of contest" # 2 in preceding section). The results are summarized in Table IV below.

TABLE IV
Threshold Histories for Initial Iteration
(*a priori* un-biased *vs.* uniform-biased)

# States	Un-biased	Uniform-biased
2	100	10
3	1,000	10
4	100,000	100
5	100,000	100
6	10,000,000	1,000

The striking results in Table IV support the conjecture that the *tendency* to inspect all states has the *tendency* to avoid FL.

4. Diagnostics

Having *easily* demonstrated FL, and investigated a strategy that *tends* to avoid it, it must be noted that we are not aware of any guarantee that FL can *always* be precluded. Despite extensive efforts by many investigators over the years, we have always encountered situations that have stymied our best FL traps in non-adaptive Monte Carlo. That is, no matter how meticulous the prescription for forming valid confidence intervals, there seem to be pathological scenarios that escape detection.

Thus, taking a cue from non-adaptive Monte Carlo methods, it would seem profitable to seek some mechanisms for diagnosing the presence of FL in adaptive Monte Carlo methods. The garden-variety of FL should be identifiable, though pathological FL will likely prevail.

A logical starting point for developing a diagnostic algorithm is consideration of a prerequisite issue, namely, identifying its desired attributes. For an FL diagnostic flag, some of its attributes are that it:

- be a true indicator of FL presence;†
  - ideally, appear in FL presence and vanish in FL absence;
  - less-than-ideally, have diminished magnitude in FL absence;

† This is a tautology, but its specification is important.

- be succinct (for easy comprehension); one number or a small set, such as the MCNP™ statistical tests;[8]
- be computable without undue diversion of resources from the main purpose of the calculation.

Recall that FL is introduced when scoring-transitions are undersampled. Moreover, FL is enhanced when the undersampled-scoring is relatively large. This suggests a basis for an FL flag:

> **Comparison between computed and theoretical values of state-to-state branching fractions, weighted by the associated scores.**

This suggested basis for an FL diagnostic flag is a recognition that, although the global solution is unknown, local behavior is known.

4.1 Proposed definition of an FL diagnostic flag

Let $\mathcal{S}_{est}$ be the estimated quantity

$$\mathcal{S}_{est} = \sum_{i=1}^{n}\sum_{j=0}^{n}\left(\frac{b_{ij}s_{ij}}{w_i}\right) \tag{4}$$

Let $\mathcal{S}_{kwn}$ be the known quantity

$$\mathcal{S}_{kwn} = \sum_{i=1}^{n}\sum_{j=0}^{n} p_{ij}s_{ij} \tag{5}$$

Then we define an FL $flag$ to be

$$flag = 1 - \frac{\mathcal{S}_{est}}{\mathcal{S}_{kwn}} \tag{6}$$

where

n is the number of discrete states (state$_0$ is the graveyard);

w_i is the total weight entering state$_i$;

b_{ij} is the weight branching from state$_i$ to state$_j$;

p_{ij} is the transition probability from state$_i$ to state$_j$;

s_{ij} is the associated score;

and $i \neq k$ for $w_k = 0$. Note that the flag is a single computed quantity, independent of n. Also, the flag vanishes for $\mathcal{S}_{est} = \mathcal{S}_{kwn}$, which is unlikely in the presence of FL, for a small number of non-zero s_{ij}.

MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory.

4.2 Test of proposed FL flag

We consider the following definition for Scenario 1:

- tight coupling between contiguous states;
- source in $state_1$; graveyard in $state_0$;
- termination probability $p_{i0} = .4$ in all $states_i$;
- transition (to nearest neighbor) probability $p_{j,j-1} = p_{j,j+1} = .3$ for interior states;
- transition probability $p_{12} = p_{n,n-1} = .6$ for end states;
- score $s_{n0} = 1$ for termination in highest $state_n$;

where n varies from 2 to 8 in this test.

The results for the above defined set of calculations are presented in Table V below. The so-called "machine epsilon," is given by Equation 3, *viz.*

$$\epsilon = 2.2 \times 10^{-16}$$

which is the (double) precision of the benchmark analytic calculations. The columns giving the results for $state_m$ correspond to the results having the maximum computed % relative error in each case.

TABLE V
Diagnostic Flag Results – Scenario 1

n states	$state_1$		$state_m$		$state_n$		flag
	mean	error [%]	mean	error [%]	mean	error [%]	
2	0.37500	$\pm$ .005	0.62500	$\pm$ .01	0.62500	$\pm$ .01	+ .02
analytic	0.374999...	ϵ	0.624999...	ϵ	0.624999...	ϵ	
3	0.11250	$\pm$ .01	0.51251	$\pm$ .02	0.51251	$\pm$ .02	− .02
analytic	0.112499...	ϵ	0.512499...	ϵ	0.512499...	ϵ	
4	0.037088	$\pm$ .009	0.16896	$\pm$ .01	0.50137	$\pm$ .004	+ .01
analytic	0.0370879...	ϵ	0.168956...	ϵ	0.501373...	ϵ	
5	0.012347	$\pm$ .01	0.012347	$\pm$ .01	0.50015	$\pm$ .002	− .0003
analytic	0.0123475...	ϵ	0.0123475...	ϵ	0.500152...	ϵ	
6	0.0041153	$\pm$ .008	0.55633	$\pm$ .01	0.50002	$\pm$ .01	− .02
analytic	0.00411529...	ϵ	0.556327...	ϵ	0.500016...	ϵ	
7	0.0013717	$\pm$ .009	0.62490	$\pm$ .02	0.50000	$\pm$ .03	+ .01
analytic	0.00137174...	ϵ	0.624905...	ϵ	0.500000...	ϵ	
8	0.00045725	$\pm$ .008	0.61813	$\pm$ .01	0.500000	$\pm$ .002	− .02
analytic	0.000457250...	ϵ	0.618130...	ϵ	0.5000000...	ϵ	

The results in Table V are indicative of proper convergence (absence of FL). The testbed results are confirmed by the analytic values. The flag behavior is seen to fluctuate about zero, with a magnitude on the order of the % relative errors for the means of state$_m$. The latter does not imply a theoretical interpretation; it is merely offered as a convenient reference for such dimensionless quantities.

We modify Scenario 1, by changing specification of state$_n$, to establish Scenario 2. The latter will encourage an FL situation:

- termination probability $p_{n0} = .999$;
- transition (to lower neighbor) probability $p_{n,n-1} = .001$;
- score for transition $s_{n,n-1} = 400$.

The results for Scenario 2, as defined above, are presented in Table VI below.

TABLE VI
Diagnostic Flag Results – Scenario 2

n states	state$_1$		state$_m$		state$_n$		flag
	mean	error [%]	mean	error [%]	mean	error [%]	
2	0.40000	± .02	0.40000	± .02	no estimate	N/A	+ .5
analytic	0.640384...	ϵ	0.640384...	ϵ	0.400640...	ϵ	
3	0.48780	± .02	0.14634	± .01	no estimate	N/A	+ .5
analytic	0.575674...	ϵ	0.292790...	ϵ	0.400292...	ϵ	
4	0.49863	± .005	0.16438	± .01	no estimate	N/A	+ .5
analytic	0.528232...	ϵ	0.213721...	ϵ	0.400184...	ϵ	
5	0.49984	± .003	0.548612	± .01	no estimate	N/A	+ .5
analytic	0.509726...	ϵ	0.9986447...	ϵ	0.4001500...	ϵ	
6	0.500000	± .0006	0.16663	± .01	no estimate	N/A	+ .5
analytic	0.5032763...	ϵ	0.172127...	ϵ	0.400138...	ϵ	
7	0.500000	± .0003	0.6098	± .03	no estimate	N/A	+ .5
analytic	0.5010958...	ϵ	0.50562...	ϵ	0.400135...	ϵ	
8	0.5000002	± .00006	0.18296	± .01	no estimate	N/A	+ .5
analytic	0.50036571...	ϵ	0.046492...	ϵ	0.400133...	ϵ	

Finally, we modify Scenario 2, by using *a priori* uniform biasing, to establish Scenario 3. The latter will tend to avoid the FL inherent in Scenario 2. The results for Scenario 3 are presented in Table VII below.

TABLE VII
Diagnostic Flag Results – Scenario 3

n states	$state_1$		$state_m$		$state_n$		flag
	mean	error [%]	mean	error [%]	mean	error [%]	
2	0.64038	$\pm$ .01	0.64038	$\pm$ .01	0.40064	$\pm$ .009	$-$ .002
analytic	0.640384...	ϵ	0.640384...	ϵ	0.400640...	ϵ	
3	0.57568	$\pm$ .01	0.29280	$\pm$ .01	0.40029	$\pm$ .01	$-$ .001
analytic	0.575674...	ϵ	0.292790...	ϵ	0.400292...	ϵ	
4	0.52823	$\pm$ .01	0.52823	$\pm$ .01	0.40018	$\pm$ .01	+ .001
analytic	0.528232...	ϵ	0.528232...	ϵ	0.400184...	ϵ	
5	0.50973	$\pm$ .006	0.40015	$\pm$ .02	0.40015	$\pm$ .02	$-$ .002
analytic	0.509726...	ϵ	0.400150...	ϵ	0.400150...	ϵ	
6	0.50327	$\pm$ .009	0.40014	$\pm$ .01	0.40014	$\pm$ .01	+ .006
analytic	0.503276...	ϵ	0.400138...	ϵ	0.400138...	ϵ	
7	0.50105	$\pm$ .01	0.40014	$\pm$ .02	0.40014	$\pm$ .02	$-$ .002
analytic	0.501095...	ϵ	0.400135...	ϵ	0.400135...	ϵ	
8	0.50036	$\pm$ .004	0.020985	$\pm$ .02	0.40013	$\pm$ .01	$-$ .003
analytic	0.500365...	ϵ	0.0209864...	ϵ	0.400133...	ϵ	

The results in Table VI are indicative of false convergence (presence of FL). The testbed results are manifestly different than the analytic values. The flag behavior is seen to maintain a positive value of .5, whose magnitude is significantly greater than the magnitude of the % relative errors for the means of $state_m$. Again, the latter does not imply a theoretical interpretation; it is merely offered as a convenient reference for such dimensionless quantities.

When *a priori* uniform sampling is introduced for the initial iteration (Scenario 3), the results in Table VII demonstrate the proper convergence. The testbed results are once again confirmed by the analytic values, and the flag behavior is seen to fluctuate about zero, being an order of magnitude less than the % relative errors for the means of $state_m$.

4.3 Follow-on work

FL diagnostics, based on estimates of cumulative branching fractions, will probably prove inadequate for large numbers of scoring-states. We will need to search for an alternative flag-basis that can function well, independent of the number of scoring-states. Ultimately, we need to extend the diagnostics algorithms to continuous transport scenarios.

5. Summary

Adaptive Monte Carlo transport relies on learned information to accelerate convergence to a zero-variance biasing solution. Such an iterative procedure is vulnerable to false learning. Any scheme that attempts to avoid such false learning must also avoid precluding zero-variance biasing, which may occur if the scheme is too conservative in it's treatment for undersampled domains of phase space. Hence, a delicate balance between the requisite convergence rate and the all-important correct result must be struck.

This investigation has demonstrated instances of FL, which lead to manifestly incorrect results. It is straightforward to contrive such a scenario, for zero-variance biasing (Equation 1), *viz.*

$$q_{ij} = C_i p_{ij}(s_{ij} + m_j)$$

as follows:

- Specify a significant score, s_{jk},
- for only one low-probability transition from state$_j$, $p_{jk} \ll 1$,
- so as to effect an initial-estimate of $m_j = 0$,
- for state$_j$,
- which has no associated score upon entry from all state$_i$, $s_{ij} = 0$,
- whereby $q_{ij} = 0$ (constituting FL), which leads to false convergence.

We have also noted some evidence that the tendency to inspect all states has the tendency to avoid FL. And we have identified a potential basis for diagnosing the presence of false learning, namely, a comparison between theoretical and computed values of quantities related to local behavior. Such comparisons are based on the recognition that, although the global solution is unknown, local behavior is known.

These findings have been based on algorithms applied to discrete state Monte Carlo transport scenarios. Follow-on efforts will strive toward eventual extension to continuous transport applications.

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